Quantification of Uncertainty in Extreme Scale compuTations

QUEST – The SciDAC UQ Institute
www.quest-scidac.org

Uncertainty Quantification (UQ) is needed for model validation and assessment of confidence in computational predictions.

UQ is a key technology for enhanced discovery from extreme scale scientific computations.

QUEST develops UQ tools for extreme scale computations and partners with science applications to apply UQ in their domains.

QUEST is a collaboration among 6 institutions

Habib N. Najm, Director
Bert J. Debusschere, Michael S. Eldred, John Jakeman
Cosmin Safta, Khachik Sargsyan, Kenny Chowdhary
SANDIA NATIONAL LABORATORIES

David M. Higdon, PI
James R. Gattiker
LOS ALAMOS NATIONAL LABORATORY

Roger G. Ghanem, PI
UNIVERSITY OF SOUTHERN CALIFORNIA

Omar Ghattas, PI
Robert Moser, Chris Simmons, Alen Alexanderian
Tan Bui-Thanh, Naomi Petra, George Stadler
THE UNIVERSITY OF TEXAS AT AUSTIN

Omar M. Knio, PI
Olivier Le Maître, Justin Winokur, Francesco RIzzi
DUKE UNIVERSITY

Youssef M. Marzouk, PI
Patrick R. Conrad, Tiangang Cui, Alex A. Gorodetsky
MASSACHUSETTS INSTITUTE OF TECHNOLOGY

Contact:

Habib N. Najm
Sandia National Laboratories
P.O.Box 969, MS 9051
Livermore, CA 94551
Tel: +1-925-294-2054
Email: hnnajm@sandia.gov

QUEST is a SciDAC Institute that is focused on uncertainty quantification (UQ) in extreme-scale scientific computations. Our goals are to (1) advance the state of the art in UQ math, algorithms, and software targetting large scale problems, and (2) provide modeling, algorithmic, and general UQ expertise, together with software tools, to other SciDAC projects, thereby enabling and guiding a broad range of UQ activities in their respective contexts.

Our vision encompasses all aspects of UQ in leadership-class computing. This includes the characterization of the input space given available data/information; local and global sensitivity analysis; adaptive dimensionality and order reduction; forward and inverse propagation of uncertainty; handling of missing data; fault tolerance; and model inadequacy, comparison, validation, selection, and averaging. The nature of the UQ problem requires the seamless combination of data, models, and information across this landscape in a manner that provides a self-consistent quantification of requisite uncertainties in predictions from computational models. Accordingly, our UQ methods and tools span an interdisciplinary space across applied math, information theory, and statistics.

UQ has a significant impact on the utility of extreme scale computations for scientific discovery. It implicitly brings in an emphasis on the quality of information available on models and their inputs, and on the use of observational data to provide well-founded estimates of uncertain inputs. This provides a solid grounding of computations in available data as well as a focus on model validation. Furthermore, UQ provides direct estimation of global sensitivity of model outputs to model inputs. This provides key information about the role of different elements of the model in impacting specific quantities of interest. This type of parametric study inherently promotes a better understanding of the meaning of the results, in a manner that a single largest-run that fits on the machine does not do. Further, it provides crucial guidance for experimental design, identifying the model inputs where additional measurements can have the highest impact in reducing uncertainty in predictions.

QUEST Software Products

We provide a number of UQ software tools that are targeted at DOE science problems. Key UQ libraries that are included in the QUEST universe are:

- DAKOTA (dakota.sandia.gov) provides a variety of non-intrusive algorithms for design optimization, model calibration, uncertainty quantification, global sensitivity analysis, solution verification, and parameter studies. It can be used as either a stand-alone application or as a set of library services.
- UQTk (www.sandia.gov/UQToolkit) is a collection of C++ libraries, and Matlab toolboxes for intrusive and non-intrusive uncertainty propagation with Polynomial Chaos expansions. It also offers C++ libraries for Markov chain Monte Carlo (MCMC) sampling in inverse problems. UQTk is primarily intended for algorithmic developments in UQ as well as educational purposes.
- QUESO (github.com/libqueso/queso) is an MPI/C++ library that provides statistical algorithms for Bayesian inference, model calibration, model validation, and decision making under uncertainty. With its foundation as a statistical UQ library, the software design maps the mathematical entities present in stochastic problems and solution methods into C++ classes, thus enabling customization and applicability to a variety of scientific domains.
- GPMSA focuses on Bayesian inference, using a Gaussian process response surface, trained from an ensemble of forward model runs, to minimize the number of forward model calls required in the inference. It allows for global sensitivity analysis, forward propagation of uncertainty, model calibration/parameter estimation, and predictions with uncertainty.
- MUQ (bitbucket.org/mituq/muq) is a C++ research library for inverse and forward UQ, with an emphasis on problem integration and an advanced modular software architecture. Core functionalities include adaptive approximations for forward UQ with large-scale models, coupled with MCMC samplers and variational approaches for model calibration and inverse problems.

Moreover, the use of UQ methods for model calibration and parameter estimation provides means of estimation of model structural error in targeted model elements, thereby enabling the identification of the specific model component that can best explain observed discrepancies with observations. Finally, recalling that the scientific method relies principally on the formulation and testing of hypotheses, and that hypothesis testing relies on statistical significance testing under conditions of sparse-data, noise, and uncertainty, it is quite clear that UQ methods for model selection and hypothesis testing are of key value for scientific discovery. This is particularly so for computations of large-scale complex physical systems, such as climate, energy, and high-energy physics, at the cutting edge of DOE/SC research, and of high relevance for DOE, where data-sparsity and uncertainties frequently render confirmation of research findings a matter of signficant complexity requiring well-founded statistical analysis. Given the significant investment of funds and resources in the DOE/SC extreme-scale computing enterprise, these various avenues by which UQ methods enhance the value of computations of systems of high relevance to DOE provide ample motivation for UQ in SciDAC.

We work collaboratively, via SC Application Partnerships, with SciDAC application projects on the use of UQ in their domains. In this context, we help partner projects in the use of QUEST tools, and to adapt the tools accordingly as needed. Both UQ and QUEST are new to SciDAC, not being part of the SciDAC universe in its earlier phases. Moreover, to a large extent, UQ is foreign to most computational scientists. Accordingly, we spend significant time and effort in each partnership project, educating application partnership researchers on what UQ is, and what it can, or cannot, do for them. Through these discussions, we have impacted the way they make use of data, and have encouraged due diligence regarding the provenance of information on model inputs, focusing attention to the upstream processing of data leading to model inputs. We are involved in 8 ongoing partnership projects, involving 5 offices within DOE/SC, including 2 partnerships with Fusion Energy Sciences, 2 with Biological and Environmental Research, 1 with Nuclear Physics, 2 with High Energy Physics, and 1 with Basic Energy Sciences.

We also conduct periodic tutorials and short courses on various aspects of the UQ problem, and our associated software tools. We have done these both as dedicated events, or as part of technical conferences. We also host an annual UQ summer school at USC, which includes both introductory lectures and talks on advanced topics given by leading invited speakers.

Further detail on the above and other information on QUEST may be found at www.quest-scidac.org.